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# Stellingen

Behorende bij het proefschrift

## Spin crossover mechanisms unraveled by theory Towards the design of new materials

Andrii Rudavskyi

1. The high spin – low spin energy difference and related parameters of thermal spin crossover can be sufficiently well described with multi-configurational methods such as CASSCF/CASPT2, given that the correct geometry of the complex is used (Chapter 3).
2. Ligand rotations caused by crystal packing are crucial for the existence of the thermal spin crossover in crystalline  $\text{Fe}(\text{mtz})_6(\text{BF}_4)_2$  (mtz = 1-methyltetrazole).  $[\text{Fe}(\text{mtz})_6]^{2+}$  ions in solution should behave as high spin complexes. This should be possible to check experimentally (Chapter 3).
3. Triplet ligand field states do play a role as intermediate states in the deactivation of the optically excited singlet states in the light-induced excited spin state trapping process in Fe(II)-based spin crossover materials (Chapter 4).
4. Increasing the ligand denticity is a promising strategy for the increase of the LIESST temperature and of the lifetimes of the metastable states.  
J.-F. Letard, G. Chastanet, P. Guionneau, C. Desplanches, in "Spin-crossover materials. Properties and applications", Ed. M. A. Halcrow, 2013; S. Hayami, Z. Gu, Y. Einaga, Y. Kobayasi, Y. Ishikawa, Y. Yamada, A. Fujishima, and O. Sato, Inorg. Chem., 2001. **40**: p. 3240-3242.
5. A moderate daily intake of Belgian beer with high alcohol content is beneficial for preventing bone fractures.  
J. Schoelynck, O. Beauchard, S. Jacobs, K. Bal, L. Barão, A. Smis, J. Van Bergen, F. Vandevenne, P. Meire, T. Van der Spiet, A. Cools, D. Van Pelt, M. J. Hodson, E. Struyf, Silicon **5**, 3, 2013.
6. Much of chemistry is theoretical, but the fun is real.  
Adapted from Sheldon Cooper, The Big Bang Theory, CBS channel.
7. Installation of a centralized system of coffee machines confirmed the hypothesis that the requirement of the high quality of products is not a priority as long as the supply is free of charge.
8. Because of their splendid architecture, spin crossover complexes can be used for contactless treatment of patients with severe Arachnophobia.  
L. C. Granado, R. Ranvaud, J. R. Peláez, Neural Plasticity, 10241, 2007.
9. Suppose that for some reason the whole scientific community of the World has suddenly vanished, such that no direct transfer of knowledge from it to those who remained was possible. Then the new generations pursuing restoration of knowledge would have to start from scratch since all published material, left from the previous scientific community, would have to be regarded as not more informative than the ancient texts, at least at the initial stage.